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Multi-scale prediction of the effective chloride diffusion coefficient of concrete

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ABSTRACT

The N-layered spherical inclusion theory is applied to develop a multi-scale model to predict the effective diffusion coefficient of chloride ion in concrete. The model treats concrete as four-phase composite materials consisting of matrix phase, aggregate phase, ITZ (interfacial transition zone) and their homogenization phase. With hardened cement pastes characterized by three parameters such as the porosity, tortuosity and constrictivity, the effect of the cement paste microstructures and ITZ on the chloride diffusivity in concrete is taken into account and the porosity distribution function and effective chloride diffusion coefficients of the ITZ are given in the model based on the cement particle distribution characteristics of the ITZ in concrete. To validate the proposed model, the diffusion coefficient of chloride ion by the steady-state migration test is measured on a series of mortar and concrete specimens and good agreement between the model and experiment is obtained. In addition, the model predicts that the chloride diffusivity of concrete composite materials depends on the chloride diffusion coefficient of the matrix and ITZ, volume fraction of the aggregate and ITZ, with the volume fraction of the ITZ influenced by aggregate size distribution, the volume fraction of aggregate and thickness of the ITZ.

1. Introduction

Chloride ion diffusivity in a porous concrete material induces steel corrosion in steel-reinforced concrete and then leads to premature deterioration of concrete structures exposed to marine environment. The chloride ion diffusion coefficient is an important indicator for concrete durability. In general, it can be obtained by long-term chloride ponding tests [1] according to concrete service environment. However, this test method is too time-consuming to meet practical requirements in a timely manner. In practice, the electrochemical accelerated testing methods [2,3] are widely used, but discrepancies occur even for identical materials due to the difference in the applied voltage, sample thicknesses and other experimental conditions.

The chloride diffusivity coefficient is also affected by the material microstructures, among which the interfacial transition zone (ITZ) between aggregates and bulk cement pastes as well as the microstructure of the cement paste itself (e.g. porosity and pore structure), are mostly dominant. A relatively reliable model to predict the chloride diffusivity coefficient should take into account concrete microstructural parameters at different scales ranging from nanometers to millimeters. Multi-scale modeling methods [4] offer a promising solution to this hard task.

The objective of the current paper is to propose a simple model to predict the chloride diffusivity based on concrete microstructures at different length scales. The key feature of the model is to take into account the ITZ and the bulk cement paste through a multi-scale approach where concrete is treated as a four-phase composite material consisting of bulk cement paste phase, aggregate phase, ITZ and their homogenization phase at mesoscopic scale. A series of mortar and concrete specimens are tested to verify the proposed model.

2. Representation of the multi-scale microstructure in concrete

Concrete is a fairly complex heterogeneous composite material, with a random microstructure at different length scales ranging from the nanometer scale to the macroscopic decimeter scale. For chloride ion diffusion problems the microstructure can be broken down into three elementary scales in this paper, according to the published literature [5,6], as sketched in Fig. 1.

– The microscopic scale (10^{-9}–10^{-6} m) mainly takes into account the pore features of hardened cement paste, which is composed of amorphous C–S–H, together with unhydrated cement products, capillary pores, crystalline calcium hydroxide, grains of submicroscopic calcium sulfoaluminate hydrate crystals and

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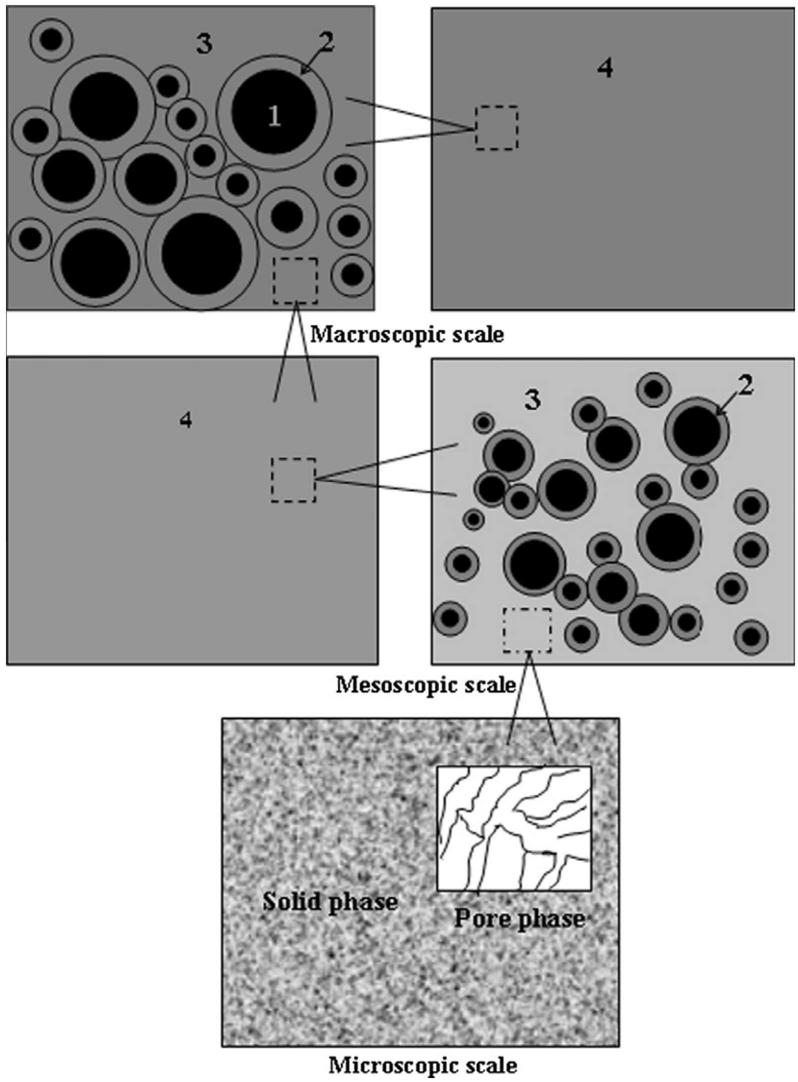

Fig. 1. Scales partition for concrete microstructure.

macroporosity in the case of high water-to-cement ratio materials. At this scale, these pores can be characterized by three parameters such as the porosity, tortuosity and constrictivity, and therefore the effective diffusion coefficient of chloride ion (D^{eff}) can be expressed as the following form:

$$D^{eff} = f(D_0, \phi_{cap}, \tau, \delta$$

where D_0 is diffusion coefficient of chloride ion in bulk water and ϕ_{cap} is capillary porosity, while τ and δ are tortuosity and constrictivity of pore structure.

– The mesoscopic scale (10^{-6}–10^{-3} m) corresponds to a 'theoretically homogeneous' material including cement paste and aggregates. At this scale, mortar may be considered as a four-phase composite material composed of aggregate phase, ITZ phase, cement matrix and their homogenization phase, corresponding to 1, 2, 3 and 4, respectively, in Fig. 1. So the effective diffusion coefficient of chloride ion (D^{eff}) can be given as the following form:

$$D^{eff} = f(D_a, V_a, D_B, D_I, V_I)$$

where V_a and V_I are volume fraction of aggregate and ITZ, respectively, while D_a, D_B and D_I are chloride diffusion coefficient of aggregate, bulk cement paste and ITZ, respectively.

– The macroscopic scale (10^{-2}–10^{-1} m) corresponds to concrete as a composite material composed of coarse aggregates embedded in a continuous homogeneous mortar matrix and an ITZ. At this scale, the estimation of effective diffusion coefficient is similar to the modeling of mesoscopic scale. The concrete is also treated as a four-phase composite material composed of aggregate phase, ITZ phase, mortar matrix and theirs homogenization phase, corresponding to 1, 2, 3 and 4, respectively in Fig. 1.

3. Transport model of chloride ion in concrete

3.1. Geometric model selection of concrete

For the sake of solving the effective diffusion coefficient in concrete, a geometry model is firstly introduced into this paper and the geometry morphology of model is required as much as possible to approach that of actual materials. Generally speaking, the composite materials could not be simply described by a single geometry model. As the introduction mentioned above, the composition and the microstructure of concrete are quite complex at different scales, and therefore it can not be simply treated as two-phase composite materials. In this paper, the composite spheres geometry model proposed by Hashin [7] is adopted to model concrete structure as depicted in Fig. 2 (two-dimensional plane). It can be